Methyl pivalate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.55

Global applicability domain: Inside

Local applicability domain index: 5.73e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

Image not found

Triethylamine
Measured: 4.90
Predicted: 5.95

Image not found

Methyl tert-butyl ether
Measured: 1.51
Predicted: 3.67

Image not found

Paraldehyde
Measured: 3.02
Predicted: 2.77

Image not found

N,N-Dimethyl-1,2-dithiolan-4-amine
Measured: 52.5
Predicted: 17.5

Image not found

4-Isobutylmorpholine
Measured: 1.78
Predicted: 2.69